Finite temperature many-particle theory of condensed matter systems in the functional Schrödinger picture

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Abstract

A finite temperature many-particle theory of condensed matter systems is formulated using the functional Schrödinger picture. Using the interacting electron gas as a model system, we solve the equation of motion for the density matrix variationally with a Gaussian type trial density matrix. We show that the present formalism yields the finite temperature Hartree-Fock results both for the para- and ferromagnetic states in a simple and convenient fashion. Implications of the present results and future prospects are also discussed.

PACS numbers : 71.10.+x,74.20.Fg,75.40.Cx

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I. INTRODUCTION

The many particle systems at finite temperatures are generally studied using the temperature Green's function through either diagrammatic or functional integral approach [1–3]. This Green's function method utilizes the Heisenberg picture and enables us to evaluate the equilibrium and nonequilibrium thermodynamic properties of systems such as the free energy and the linear responses when perturbative expansions are available. On the other hand, the Schrödinger picture, which is a more familiar concept in quantum mechanics has not been much used in the many-body theory, although the usefulness of this picture for the study of quantum structures of field theories was recognized early by several authors [4–6]. Only recently, it has been shown that a many-particle theory of condensed matter systems can be successfully formulated using the functional Schrödinger picture(FSP) [7]. However, the theory was limited to the zero-temperature and, thus, requires extension to finite temperature to be truly useful for many-particle studies.

In this paper, we present a finite temperature formulation of many-particle theory based on the functional Schrödinger picture. We apply the theory on the interacting electron gas system and show that a Gaussian approximation of the theory produces the finite temperature Hartree-Fock results both for the para- and ferromagnetic phases in a simple and convenient fashion. We also show that the self-consistent equation for the ferromagnetic splitting yields the Stoner criterion for the ferromagnetism.

II. NON-INTERACTING ELECTRON GAS SYSTEM

A finite temperature quantum field theory using the functional Schrödinger picture has been recently formulated [8,9] by generalizing the Gaussian approximation of the variational calculation in quantum mechanics [10]. The method is based on the Feynman's observation that the unnormalized density matrix

$$\rho = e^{-\beta H} \tag{1}$$

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satisfies the equation

$$-\frac{\partial \rho}{\partial \beta} = H\rho , \tag{2}$$

where β is the inverse temperature and H the Hamiltonian of the system [11].

First, we study the non-interacting particle system which has the grand Hamiltonian given by

$$\begin{aligned}
\hat{K} &= \hat{H} - \mu \hat{N} \\
&= \sum_\alpha \int d^3x \psi_\alpha^\dagger(\vec{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 \right] \psi_\alpha(\vec{x}) - \mu \hat{N} ,
\end{aligned} \tag{3}$$

where $\hat{N}$ represents the number operator and μ the chemical potential. In the FSP, the fermion field operator ψ and its conjugate momentum $i\psi^\dagger$ are expressed as functional operators. Following the Floreanini-Jackiw prescription [12], the fermionic field operators are expressed as

$$\begin{aligned}
\psi(x) &= \frac{1}{\sqrt{2}} \left[u(x) + \frac{\delta}{\delta u(x)^\dagger} \right] , \\
\psi^\dagger(x) &= \frac{1}{\sqrt{2}} \left[u(x)^\dagger + \frac{\delta}{\delta u(x)} \right]
\end{aligned} \tag{4}$$

to satisfy the equal-time anticommutation relation $\{\psi_i(x,t), \ \psi_j^\dagger(x',t)\} = \delta_{ij}\delta(x-x')$, where u and $u^\dagger$ are anticommuting Grassmann variables. Using the above expressions, we rewrite the grand Hamiltonian as follows,

$$\hat{K} = \frac{1}{2} \sum_{A,B} \xi_{AB} \left(u_A^\dagger + \frac{\delta}{\delta u_A} \right) \left(u_B + \frac{\delta}{\delta u_B^\dagger} \right) , \tag{5}$$

where $\xi_{AB} = -\frac{\hbar^2}{2m} [\delta(\vec{x}-\vec{y})\nabla_y^2]\delta_{\alpha\beta} - \mu\delta_{AB}$ and $A = (\vec{x},\alpha),\ B = (\vec{y},\beta)$. We choose a Gaussian trial density matrix

$$\rho = e^{u_A^\dagger F_{AB} u_B + J_A u_A + u_A^\dagger L_A + C} , \tag{6}$$

to satisfy the differential equation,

$$-\frac{\partial \rho}{\partial \beta} = K\rho . \tag{7}$$

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Substituting Eq.(6) into Eq.(7), we obtain the following identity equation,

$$-u^\dagger \frac{\partial F}{\partial \beta} u - \frac{\partial J}{\partial \beta} u - u^\dagger \frac{\partial L}{\partial \beta} - \frac{\partial C}{\partial \beta} = \frac{1}{2} \Big[u^\dagger (\xi - F\xi F) u + u^\dagger (\xi L - F\xi L)$$

$$+ (-J\xi - J\xi F) u + (\xi + F\xi - J\xi L) \Big] . \tag{8}$$

Since the above equation is an identity equation with respect to u and $u^\dagger$, we obtain four differential equations. The four equations are readily solved to yield

$$F = -coth(\frac{1}{2}\beta\xi) , \tag{9}$$

$$J = -v^\dagger e^{\frac{1}{2}\beta\xi} [sinh(\frac{1}{2}\beta\xi)]^{-1} , \tag{10}$$

$$L = -v e^{-\frac{1}{2}\beta\xi} [sinh(\frac{1}{2}\beta\xi)]^{-1} , \tag{11}$$

$$C = Tr\Big[-\frac{1}{2}\beta\xi + ln[sinh(\frac{1}{2}\beta\xi)] - v^\dagger v coth(\frac{1}{2}\beta\xi) \Big] . \tag{12}$$

In the above, Grassmann variables v and $v^\dagger$ are introduced as constants of integrations in order to make ρ a Gaussian type density matrix [8]. The normalized density matrix is obtained using these relations,

$$\rho_{nor} = \frac{1}{\mathcal{N}} e^{Tr[-\frac{1}{2}\beta\xi]} Det[sinh(\frac{1}{2}\beta\xi)] e^{u^\dagger v - v^\dagger u} e^{-(u^\dagger + v^\dagger)[coth(\frac{1}{2}\beta\xi)](u+v)} , \tag{13}$$

where the normalization constant $\mathcal{N}$ is obtained by the relation, $1 = Tr[\rho_{nor}]$,

$$\mathcal{N} = e^{Tr[-\frac{1}{2}\beta\xi]} Det[4 cosh \frac{1}{2}\beta\xi] . \tag{14}$$

This normalized density operator corresponding to the above normalized density matrix is given by

$$\hat{\rho}_{nor} = \frac{e^{Tr[\frac{1}{2}\beta\xi]}}{Det[4 cosh(\frac{1}{2}\beta\xi)]} e^{-\beta\hat{K}} . \tag{15}$$

The Helmholtz free energy is defined by

$$\beta F \equiv < ln\hat{\rho}_{nor} > + \beta < H > . \tag{16}$$

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Substituting Eq.(15) into Eq.(16) and using Eq.(13) to calculate the expectation value, we obtain

$$F = N\mu - k_B T \ Tr[ln(1 + e^{-\beta\xi})] - Tr[ln2] \ . \tag{17}$$

The Fourier transformation of the above equation gives the familar result as follows,

$$F = N\mu - k_B T \ \sum_{k,\sigma}[ln(1 + e^{-\beta\xi_k})] - Nln2 \ , \tag{18}$$

where $\xi_k \equiv \epsilon_k^0 - \mu \equiv \frac{\hbar^2 k^2}{2m} - \mu$, and α is the spin index. The total energy is also readily obtained

$$\begin{aligned}
E &= < \hat{H} > \\
&= \sum_{A,B} \int DuDu^\dagger h_{AB}\psi_A^\dagger \psi_B \rho_{uv}|_{u=v} \\
&= \sum_{k,\sigma} \epsilon_k^0 n_k \ ,
\end{aligned} \tag{19}$$

where $h_{AB} = \xi_{AB} + \mu$ and

$$n_k = \frac{1}{1 + e^{\beta(\epsilon_k^0 - \mu)}} \ . \tag{20}$$

These results on the non-interacting electron system clearly show that a finite temperature many-particle theory can be successfully formulated using the density matrix method based on the FSP approach.

III. INTERACTING ELECTRON GAS SYSTEM

Next, we investigate the interacting electron gas system of which the grand Hamiltonian is given by

$$\hat{K} = \sum_{A,B} \xi_{AB}\hat{\psi}_A^\dagger\hat{\psi}_B + \frac{1}{2}\sum_{A,B} V_{AB}\hat{\psi}_A^\dagger\hat{\psi}_B^\dagger\hat{\psi}_B\hat{\psi}_A \ , \tag{21}$$

where V_{AB} is any appropriate particle-particle interaction potential. The density matrix for an interacting system is not a Gaussian and generally quite complex. As a first approximation, we choose a trial Gaussian density matrix with a parameter function, which will

be chosen from minimization of the thermodynamic potential. Thus, the normalized trial density matrix is given by

$$\rho_{nor} = \frac{1}{Det[4coth(\frac{1}{2}\beta Q)]}e^{u^\dagger v - v^\dagger u}e^{-(u^\dagger + v^\dagger)[coth(\frac{1}{2}\beta Q)](u+v)} , \tag{22}$$

where Q is the adjustible parameter matrix. The normalized density operator is written in the form

$$\hat{\rho}_{nor} = \frac{e^{Tr[\frac{1}{2}\beta Q]}}{Det[4cosh(\frac{1}{2}\beta Q)]}e^{-\beta\hat{\psi}^\dagger Q\hat{\psi}} , \tag{23}$$

in analogy with the free particle case. The thermodynamic potential is defined by

$$\beta\mathbf{\Omega} = \beta(F - \mu N)$$

$$= < ln\hat{\rho}_{nor} > +\beta < \hat{H} > -\beta\mu < \hat{N} >$$

$$= < ln\hat{\rho}_{nor} > +\beta < \hat{K} > . \tag{24}$$

Substituting Eq.(23) into Eq.(24), we obtain

$$\beta\mathbf{\Omega} = \frac{1}{2}\beta\sum_A Q_{AA} - \sum_A [ln[4cosh(\frac{1}{2}\beta Q)]]_{AA}$$

$$-\frac{1}{2}\beta\sum_{A,B} Q_{AB}G_{BA} + \frac{1}{2}\beta\sum_{A,B} \xi_{AB}G_{BA}$$

$$+\frac{1}{8}\beta\sum_{A,B} V_{AB}[G_{AA}G_{BB} - G_{BA}G_{AB}] , \tag{25}$$

where $G = I - tanh(\frac{1}{2}\beta Q)$, and I is the identity matrix. The Fourier transformation of the above equation is

$$\beta\mathbf{\Omega} = -V\int dKtr[ln[4coshA(\vec{k})]]$$

$$+V\int dKtr[A(\vec{k})tanhA(\vec{k})]$$

$$+\frac{1}{2}V\beta\int dKtr[\xi(\vec{k})G(\vec{k})]$$

$$+\frac{1}{8}V\beta V(0)\int dKtr[G(\vec{k})]\int dK'tr[G(\vec{k}')]$$

$$-\frac{1}{8}V\beta\int dKdK'V(\vec{k}-\vec{k}')tr[G(\vec{k})G(\vec{k}')] , \tag{26}$$

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where $A(\vec{k}) = \frac{1}{2}\beta Q(\vec{k})$, $G(\vec{k}) = \sigma_0 - tanh(\frac{1}{2}\beta Q(\vec{k}))$, tr is the trace for the spin indices only, and σ_0 is the 2×2 identity matrix. Introducing a constraint parameter N,

$$N \equiv \frac{1}{2}V \int dK tr[G(\vec{k})] , \tag{27}$$

we rewrite the thermodynamic potential as follows,

$$
\begin{aligned}
\beta\mathbf{\Omega} = {} & \alpha\Big[N - \frac{1}{2}V \int dK tr[G(\vec{k})]\Big] \\
& -V \int dK tr[ln[4 cosh A(\vec{k})]] \\
& +V \int dK tr[A(\vec{k}) tanh A(\vec{k})] \\
& +\frac{1}{2}V\beta \int dK tr[\xi(\vec{k})G(\vec{k})] \\
& +\frac{1}{2}\frac{V(0)}{V}\beta N^2 \\
& -\frac{1}{8}V\beta \int dK dK' V(\vec{k} - \vec{k}') tr[G(\vec{k})G(\vec{k}')] ,
\end{aligned}
\tag{28}
$$

where α is the Lagrange's undetermined multiplier. Taking variations on $\beta\mathbf{\Omega}$ with respect to N and $A(\vec{k})$, we obtain

$$\alpha = -\frac{V(0)}{V}\beta N , \tag{29}$$

$$\beta Q(\vec{k}) = (\beta\xi(\vec{k}) - \alpha)\sigma_0 - \frac{1}{2}\beta \int dK' V(\vec{k} - \vec{k}')G(\vec{k}') . \tag{30}$$

Eq.(30) is a self-consistent equation which determines $Q(\vec{k})$. Since all functions in the above equation are 2×2 matrices, $Q(\vec{k})$ and $G(\vec{k})$ are also represented as linear combinations of the Pauli matrices.

First, we consider the symmetry conserving paramagnetic case. In this case, the eigenvalues of $G(\vec{k})$ are same for both spins, and, thus, $Q(\vec{k})$ and $G(\vec{k})$ must be multiples of the 2×2 identity matrix,

$$Q(\vec{k}) = q(\vec{k})\sigma_0 , \tag{31}$$

$$G(\vec{k}) = g(\vec{k})\sigma_0 . \tag{32}$$

Defining $q(\vec{k}) \equiv \epsilon_k - \mu$, we can rewrite $g(\vec{k})$ as follows

$$
\begin{aligned}
g(\vec{k}) &= 1 - tanh[\frac{1}{2}\beta(\epsilon_k - \mu)] \\
&= \frac{2}{1 + e^{\beta(\epsilon_k - \mu)}} \\
&= 2n_k .
\end{aligned}
\tag{33}
$$

Here, n_k is the Fermi distribution function of the interacting system. The energy spectrum of the interacting system is obtained from Eq.(30)

$$
\epsilon_k = \epsilon_k^0 + (2S + 1)V(0)n - \int dK'V(\vec{k} - \vec{k}')n_{k'} ,
\tag{34}
$$

where $n = N/V$ is the number density. The above equation is the familiar self-consistent Hartree-Fock equation which determines the energy spectrum of the interacting electron gas system [1]. Using the above results, we readily obtain the total energy and the Helmholtz free energy

$$
E =< H >= (2S + 1)V \int dK(\epsilon_k^0 + \frac{1}{2}\Sigma_k)n_k ,
\tag{35}
$$

and

$$
\begin{aligned}
F &= \mathbf{\Omega} + N\mu \\
&= N\mu - Nk_BTln2 - k_BT(2S + 1)V \int dKln[1 + e^{-(\epsilon_k - \mu)/k_BT}] ,
\end{aligned}
\tag{36}
$$

where the self-energy Σ_k is given by

$$
\Sigma_k = (2S + 1)V(0)n - \int dK'V(\vec{k} - \vec{k}')n_{k'} .
\tag{37}
$$

Next, we consider the magnetic symmetry breaking solution. In order to represent the ferromagnetic state, we express $Q(\vec{k})$ as follows

$$
Q(\vec{k}) = (\epsilon_k - \mu)\sigma_0 + \gamma_k\sigma_3 .
\tag{38}
$$

Assuming that γ_k is much smaller than ϵ_k and expanding to the first order of γ_k, we obtain

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$$tanh\frac{1}{2}\beta\left[(\epsilon_k - \mu)\sigma_0 + \gamma_k\sigma_3\right] \approx \sigma_0 tanh\frac{1}{2}\beta(\epsilon_k - \mu) + \sigma_3\frac{1}{2}\beta\gamma_k sech^2\frac{1}{2}\beta(\epsilon_k - \mu) \ . \tag{39}$$

Using Eq.(30), Eq.(38) and (39), we obtain for the ferromagnetic state

$$\beta[(\epsilon_k - \mu)\sigma_0 + \gamma_k\sigma_3] = (\beta\xi_k - \alpha)\sigma_0 - \frac{1}{2}\int dK'V(\vec{k} - \vec{k}')\Big[\sigma_0(1 - tanh\frac{1}{2}\beta(\epsilon_{k'} - \mu))$$
$$-\sigma_3\frac{1}{2}\beta\gamma_{k'}sech^2\frac{1}{2}\beta(\epsilon_{k'} - \mu)\Big] \ . \tag{40}$$

From this identity equation, we obtain two self-consistent equations as follows,

$$\epsilon_{k\sigma} = \epsilon_0 + (2S + 1)V(0)n - \int dK'V(\vec{k} - \vec{k}')n_{k'\sigma} \ , \tag{41}$$

$$\gamma_k = \frac{1}{4}\int dK'V(\vec{k} - \vec{k}')\gamma_{k'}sech^2[\frac{1}{2}\beta(\epsilon_{k'} - \mu)] \ . \tag{42}$$

Eq.(41) shows that the one-particle energy is now dependent on the spin index. Solving Eq.(42) self-consistently, one can obtain the amount of splitting between the up- and down-energy spectrum. Also Eq.(42) yields the celebrated Stoner condition as follows

$$1 = \overline{V}(0)\int dK\left[-\frac{\partial n(\epsilon_k)}{\partial\epsilon_k}\right]$$
$$\equiv \overline{V}F(0)$$
$$\approx \overline{V}N(0) \ . \tag{43}$$

Here, $F(0)$, $N(0)$ and $\overline{V}(0)$ represent the static Lindhard function, the density of state at the Fermi surface and the average exchange interaction respectively. The total energy and the thermodynamic potential are given by

$$E = V\sum_\sigma\int dK[\epsilon_k^0 + \frac{1}{2}\Sigma_{k\sigma}]n_{k\sigma} \ , \tag{44}$$

$$\mathbf{\Omega} = -\frac{1}{\beta}ln\ 2 - \frac{1}{\beta}V\sum_\sigma\int dKln\left[1 + e^{-\beta(\epsilon_{k\sigma} - \mu)}\right] \ , \tag{45}$$

where

$$\Sigma_{k\sigma} = \frac{1}{2}V(0)n - \frac{1}{2}\int dK'V(\vec{k} - \vec{k}')n_{k'\sigma} \ ,$$
$$n_{k\sigma} = \frac{1}{1 + e^{\beta(\epsilon_{k\sigma} - \mu)}} \ . \tag{46}$$

$\epsilon_{k\sigma}$ and $n_{k\sigma}$ can be determined self-consistently once γ_k is obtained through Eq.(42).

IV. CONCLUSION

In this paper, we have presented a finite temperature many-particle theory based on the functional Schrödinger picture formalism. First, we have shown how the functional Schrödinger picture formalism can be applied to many-particle systems by solving the free-particle system exactly. Next, using the Gaussian density matrix obtained from the free-particle system, we have constructed a variational calculation formalism for the interacting electron gas system. The present variational formalism yields both the paramagnetic and the ferromagnetic solutions as in the case of the zero-temperature formalism. For the ferromagnetic state, we have obtained a self-consistent equation which determines the splitting of energy between the two spin-split states. Also this equation leads to the Stoner criterion for the ferromagnetism.

Here, we note that the above theoretical scheme is general and, thus, can be applied to any interacting condensed matter systems. Since the present theory is variational, and not perturbative, it is expected to become a useful tool for investigation of strongly correlated systems. In order to obtain results beyond the Hartree-Fock terms, it is necessary to carry out calculations beyond the Gaussian approximations. Variational methods employing non-Gaussian trial functionals and perturbational approach based on variational basis are under study and will be reported elsewhere. In conclusion, we believe that this application of the functional Schrödinger picture theory to finite temperature clearly demonstrates the versality and possible applicability of the theory to wide range of condensed matter problems.

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